# Benzoic acid, 2-hydroxy-, phenyl ester

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|---|---|
| **Other names:** | 2-Hydroxy-benzoic acid phenyl ester |
| | 2-hydroxybenzoic acid phenyl ester |
| | 2-phenoxycarbonylphenol |
| | Fenylester kyseliny salicylove |
| | NSC 33406 |
| | musol |
| | phenol salicylate |
| | phenyl 2-hydroxybenzenecarboxylate |
| | phenyl 2-hydroxybenzoate |
| | phenyl salicylate |
| | salicylic acid phenyl ester |
| | salicylic acid, phenyl ester |
| | salol |
| | salphenyl |
| | seesorb 201 |
| | seesorb K 201 |
| **Inchi:** | InChI=1S/C13H10O3/c14-12-9-5-4-8-11(12)13(15)16-10-6-2-1-3-7-10/h1-9,14H |
| **InchiKey:** | ZQBAKBUEJOMQEX-UHFFFAOYSA-N |
| **Formula:** | C13H10O3 |
| **SMILES:** | O=C(Oc1ccccc1)c1ccccc1O |
| **Mol. weight [g/mol]:** | 214.22 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chs | -6109.10 | kJ/mol | NIST Webbook |
| hf | -334.97 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 26.08 | kJ/mol | Joback Method |
| hvap | 86.29 | kJ/mol | Cheméo Relay (1.0) |
| ie | 7.97 | eV | Cheméo Relay (1.0) |
| log10ws | -3.15 | | Aqueous Solubility Prediction Method |
| logp | 2.611 | | Crippen Method |
| mcvol | 159.820 | ml/mol | McGowan Method |
| pc | 3862.67 | kPa | Joback Method |
| rinpol | 1702.00 | | NIST Webbook |
| rinpol | 1650.00 | | NIST Webbook |
| rinpol | 1655.00 | | NIST Webbook |

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|---|---|---|---|
| rinpol | 1660.00 | | NIST Webbook |
| rinpol | 1702.00 | | NIST Webbook |
| rinpol | 1650.00 | | NIST Webbook |
| rinpol | 1650.00 | | NIST Webbook |
| rinpol | 1650.00 | | NIST Webbook |
| rinpol | 1655.00 | | NIST Webbook |
| tb | 582.78 | K | Cheméo Relay (1.0) |
| tc | 888.18 | K | Cheméo Relay (1.0) |
| tf | 315.00 ± 1.50 | K | NIST Webbook |
| tf | 314.49 ± 0.20 | K | NIST Webbook |
| tf | 314.53 ± 1.00 | K | NIST Webbook |
| tf | 314.82 ± 0.20 | K | NIST Webbook |
| tf | 314.84 ± 0.20 | K | NIST Webbook |
| tf | 314.83 ± 0.25 | K | NIST Webbook |
| tf | 314.90 | K | The use of organic calibration standards in the enthalpy calibration of differential scanning calorimeters |
| tt | 314.75 | K | Investigation of the melting behavior of the reference materials biphenyl and phenyl salicylate by a new type adiabatic scanning calorimeter |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 475.68 | J/mol×K | 962.79 | Joback Method |
| cpg | 448.02 | J/mol×K | 834.95 | Joback Method |
| cpg | 457.84 | J/mol×K | 877.56 | Joback Method |
| cpg | 467.02 | J/mol×K | 920.18 | Joback Method |
| cpg | 413.44 | J/mol×K | 707.11 | Joback Method |
| cpg | 425.94 | J/mol×K | 749.72 | Joback Method |
| cpg | 437.42 | J/mol×K | 792.34 | Joback Method |
| dvisc | 0.0000885 | Pa×s | 551.03 | Joback Method |
| dvisc | 0.0001645 | Pa×s | 512.01 | Joback Method |
| dvisc | 0.0003388 | Pa×s | 472.99 | Joback Method |
| dvisc | 0.0000517 | Pa×s | 590.05 | Joback Method |
| dvisc | 0.0000323 | Pa×s | 629.07 | Joback Method |
| dvisc | 0.0000213 | Pa×s | 668.09 | Joback Method |
| dvisc | 0.0000147 | Pa×s | 707.11 | Joback Method |
| hfust | 18.98 | kJ/mol | 314.20 | NIST Webbook |

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|---|---|---|---|---|
| hfust | 18.40 ± 0.50 | kJ/mol | 312.70 | NIST Webbook |
| hfust | 19.20 | kJ/mol | 315.10 | NIST Webbook |
| hfust | 19.16 | kJ/mol | 315.00 | NIST Webbook |
| hsubt | 109.10 | kJ/mol | 297.00 | NIST Webbook |
| hvapt | 69.90 | kJ/mol | 505.00 | NIST Webbook |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 446.20 | K | 1.60 | NIST Webbook |

# Sources

**Interpretation of the global heat of melting in eutectic binary systems:** https://www.doi.org/10.1016/j.tca.2018.04.011

**Solubility of Salol in Pure Alcohols from (283.15 to 308.15) K:** https://www.doi.org/10.1021/je800668j

**KDB:** https://www.cheric.org/files/research/kdb/mol/mol1154.mol

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C118558&Units=SI

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

**Thermodynamic Study of Phenyl Salicylate Solutions in Aprotic Solvents at Different Temperatures:** https://www.doi.org/10.1021/je8003595

**Aqueous Solubility Prediction Method:** http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

**Cheméo Relay (1.0):**

**Cheméo Relay (1.0, beta):**

**Investigation of the melting behavior of the reference materials biphenyl and phenyl salicylate by a new type adiabatic scanning calorimeter:** https://www.doi.org/10.1016/j.tca.2014.02.023

**Joback Method:** https://en.wikipedia.org/wiki/Joback_method

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**The use of organic calibration standards in the enthalpy calibration of differential scanning calorimeters:** https://www.doi.org/10.1016/j.tca.2012.03.028

# Legend

**chs:** Standard solid enthalpy of combustion

**cpg:** Ideal gas heat capacity

**dvisc:** Dynamic viscosity

**hf:** Enthalpy of formation at standard conditions

**hfus:** Enthalpy of fusion at standard conditions

**hfust:** Enthalpy of fusion at a given temperature

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|---|---|
| **hsubt:** | Enthalpy of sublimation at a given temperature |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **tt:** | Triple Point Temperature |

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